

Model Performance

Model

Data

Weighted KNN model					
5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.25e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 7.55e-01

Confidence level: 7.34e-01

Nearest Neighbors from the Training Set

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<div>Image not found</div> <div>Pebulate</div> <div>Measured: 4.92e-04</div> <div>Predicted: 4.82e-04</div>	<div>Image not found</div> <div>Butylate</div> <div>Measured: 2.07e-04</div> <div>Predicted: 3.42e-04</div>	